

AMENDMENTS TO THE CLAIMS

This listing of claims will replace all prior versions, and listings, of claims in this application:

Listing of Claims

1. (Original) A method of characterizing a mixture of components, the method comprising the steps of:
 - obtaining a plurality of spectrochromatograms of the mixture of components, each of the spectrochromatograms being obtained under a respective one of a plurality of different chromatographic conditions;
 - estimating the number of components and
 - performing component matching upon the spectrochromatograms using the estimated number of components.
2. (Original) The method of claim 1 further comprising the step of determining each component retention time in response to the component matching.
3. (Original) The method of claim 1 further comprising the step of determining each component spectral shape in response to the component matching.
4. (Original) The method of claim 3 further comprising the step of using the component spectral shape to identify the component.
5. (Original) The method of claim 1 further comprising the step of resolving at least one component in the mixture of components.
6. (Original) A method of component peak matching comprising the steps of:
 - obtaining a plurality of spectrochromatographic data sets for a mixture of components, each spectrochromatographic data set comprising spectrochromatographic data;
 - creating an augmented spectrochromatographic data set by merging the spectrochromatographic data sets into a matrix;
 - determining a preliminary estimate of the number of components (n) in the augmented spectrochromatographic data set;
 - selecting the (n) most orthogonal spectrochromatographic data from the augmented spectrochromatographic data set;
 - generating a refined key spectra set; and

determining the component retention times.

7. (Original) The method of claim 6 further comprising the step of:

validating each of the (n) most orthogonal spectrochromatographic data using target factor analysis to generate the refined key spectra set.

8. (Original) The method of claim 6 further comprising the step of detecting missing components using target testing of each spectrochromatographic data in the refined key spectra set against each of the plurality of spectrochromatographic data sets.

9. (Original) The method of claim 6 wherein the step of determining a preliminary estimate uses principle component analysis.

10. (Original) The method of claim 6 wherein the step of determining a preliminary estimate uses single value decomposition.

11. (Original) The method of claim 6 wherein the step of determining a preliminary estimate uses nonlinear iterative partial least squares.

12. (Original) The method of claim 6 wherein the step of selecting the (n) most orthogonal spectra uses modified Iterative Key Set Factor Analysis.

13. (Original) The method of claim 6 wherein the step of determining the component retention times comprises:

performing a regression using the refined key spectra set and the augmented data matrix;

and

determining retention times as maximum values.

14. (Original) A method for resolving a mixed sample of chromatographic components, the method comprising the steps of:

selecting a plurality of differing chromatographic conditions;

performing a plurality of chromatographic runs on the mixed sample, each respective run performed under a respective chromatographic condition;

obtaining spectrochromatographic data for the mixed sample during each of the chromatographic runs;

creating an augmented data set from the spectrochromatographic data of the plurality of chromatographic runs;

operating on the augmented data set to determine the retention times for each component in the mixed sample; and

resolving each of the components.

15. (Original) The method of claim 14 further comprising the step of performing component quantitation.

16. (Original) The method of claim 15 wherein the step of performing component quantitation uses resolved spectra and concentration profiles.

17. (Original) The method of claim 14 further comprising the step of finding peak relative areas using concentration profiles.

18. (Original) A method of obtaining the shape of components from spectrochromatographic data comprising the steps of:

determining the number of components (n) and each component's retention time;

generating uniqueness vectors as initial estimates of spectrochromatographic profiles; and

performing profile resolution on the spectrochromatographic data.

19. (Original) The method of claim 18 wherein the step of performing profile resolution uses ALS MCR.